Supporting Information

KFeSbTe$_3$: a quaternary chalcogenide aerogel for preferential adsorption of polarizable hydrocarbons and gases

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Supplementary Figures:

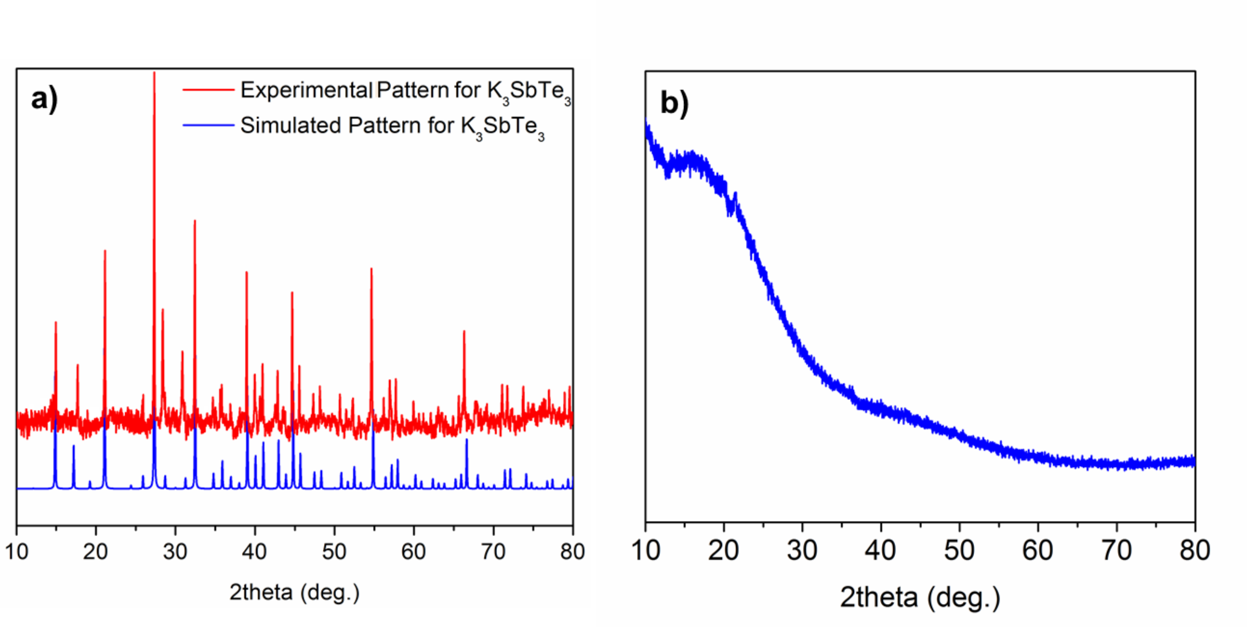
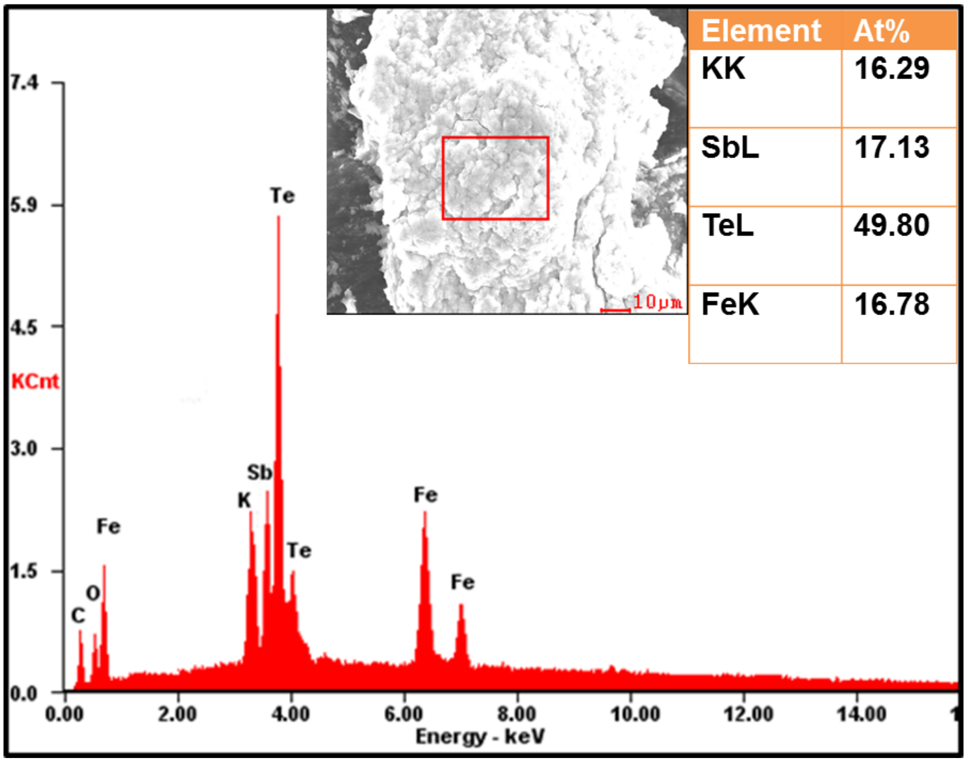


Figure S1 Powder XRD patterns; a) ternary phase K$_3$SbTe$_3$, b) predominantly amorphous nature of the aerogel KFeSbTe$_3$.



Element	At%
KK	16.29
SbL	17.13
TeL	49.80
FeK	16.78

Figure S2 EDS results of the $KFeSbTe_3$ aerogel with SEM images in the inset.

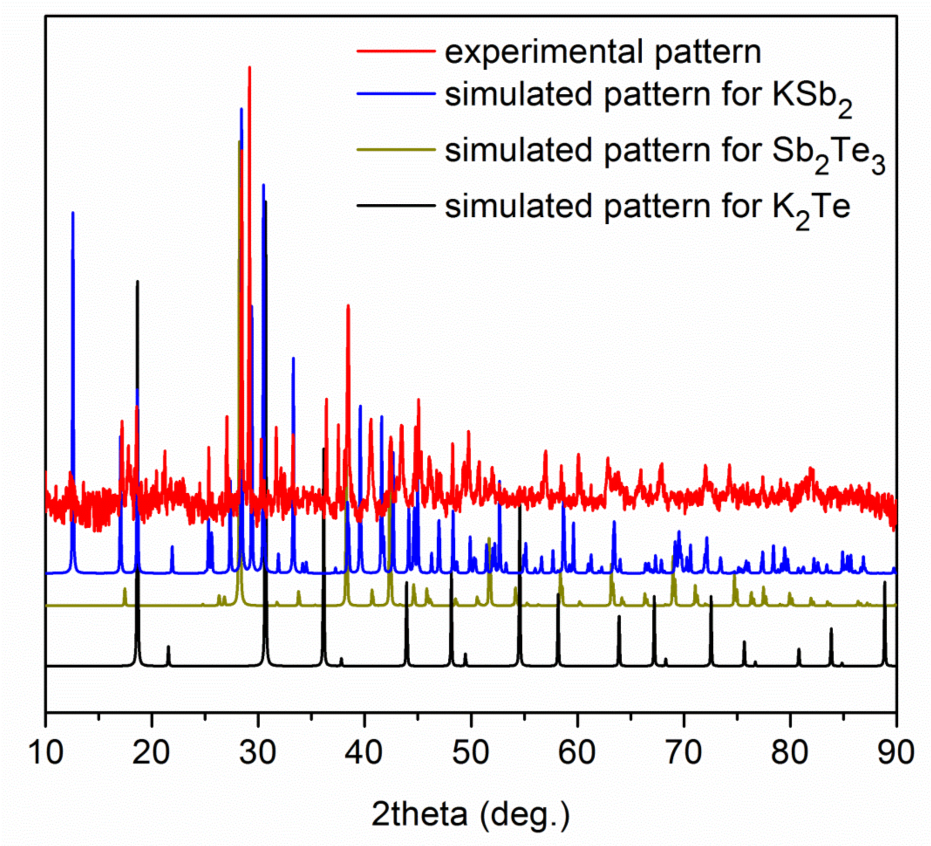


Figure S3 Powder XRD pattern of the products after the solvothermal reaction.

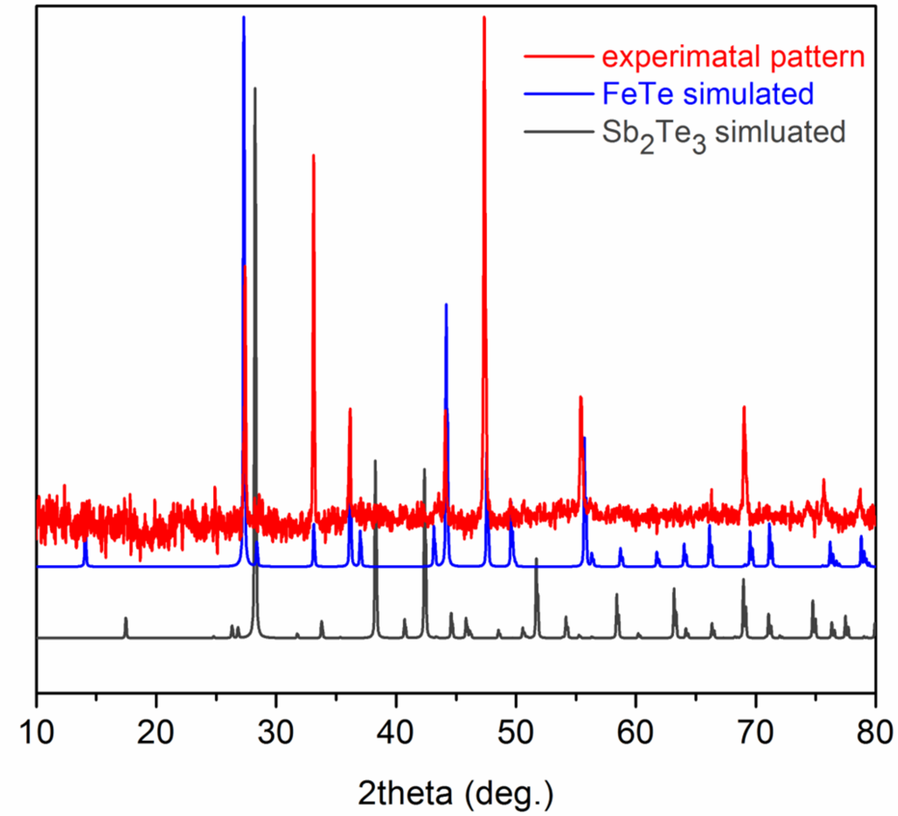


Figure S4 Powder XRD pattern of the $KFeSbTe_3$ chalcogel after TGA.

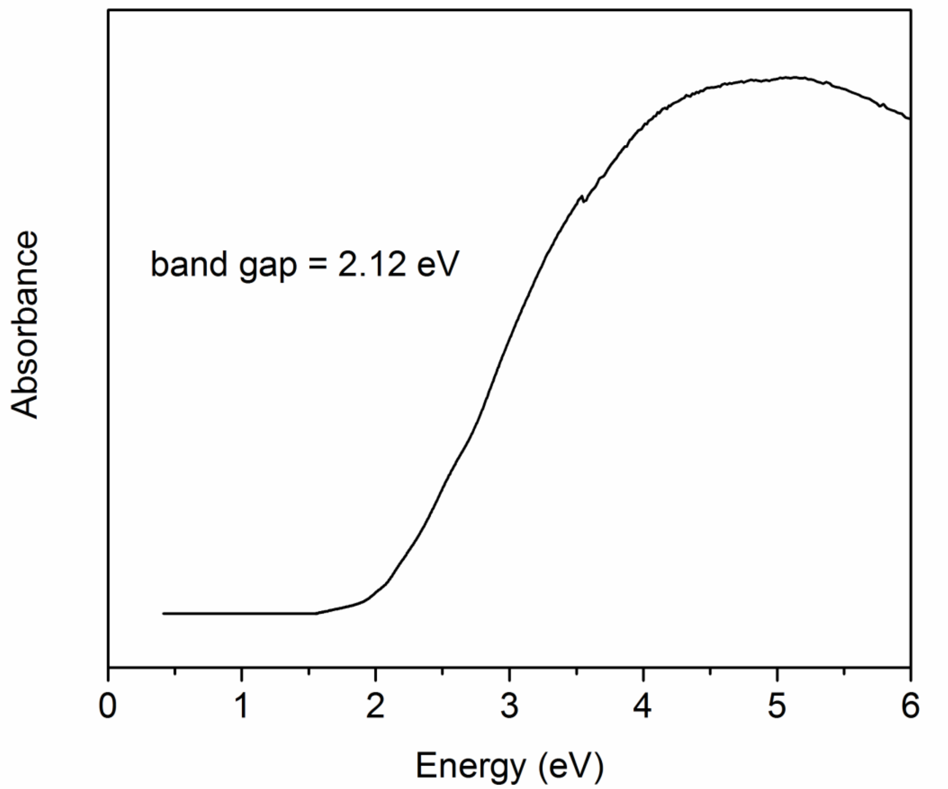


Figure S5: Solid-state UV-Vis optical absorption spectra for $KFeSbTe_3$.

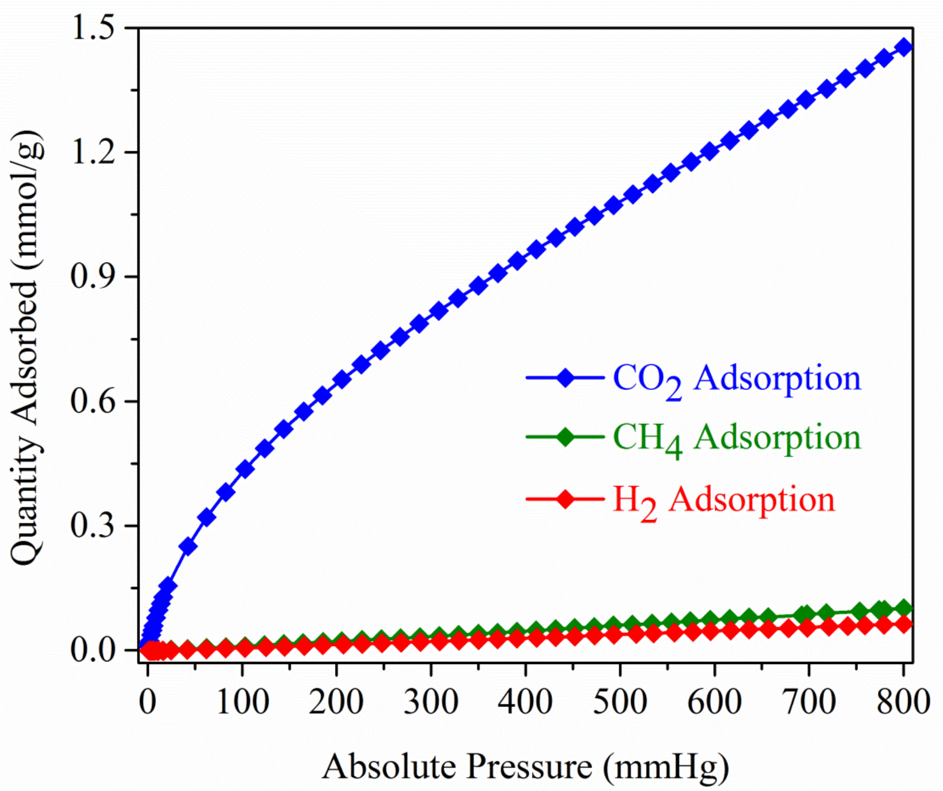


Figure S6: Adsorption isotherms of CO_2, CH_4 and H_2 observed in $KFeSbTe_3$ at 263 K.

Table S1. Comparison of Toluene adsorption capacity in different porous materials.

Adsorbent	Surface Area m^2/g	Toluene adsorption mg/g	Temperature K	Ref
MOF-177	2970	585	298	1
MIL-100(Fe)	>2000	630	303	2
ML-101	3980	1096	298	3
PCH	740	267	298	3
Y-zeolite	704	150	293	3
$Cu_3(BTC)_2$	1507	234	298	4
Activated carbon	990	109	298	5
13X-zeolite	440	16	298	5
Silica gel	535	143	298	5
$KFe_3Co_3S_{21}$	558	276	298	6
$KFe_3Y_3S_{22}$	461	119	298	6
$KFe_3Eu_3S_{22}$	573	313	298	6
$KFeSbTe_3$	652	856	293	This work

Table S2. Comparison of CO_2/H_2 and CO_2/CH_4 selectivity in different porous materials.

Adsorbent	Surface Area m^2/g	Temperature K	Selectivity CO_2/H_2, CO_2/CH_4	Ref
FAU-type zeolite	3213	298	18, NA	7
Cu-BTC	1600	298	60, 10	8
MOF-5 (IRMOF-1)	2304	296	25, 3	8
SIFSIX-2-Cu-i	735	298	33, 240	9
SIFSIX-3-Zn	250	298	>1800, 231	9
Mg_2(dobdc)	1800	313	800, NA	10
Chalcogel (Co, Ni-MoS_4)	340	273	16, NA	11
Chalcogel-Pt-1 (PtGeS)	323	273	6, NA	12
Chalcogel-PtSb-1 (PtSbGeSe)	226	273	12, NA	12
Chalcogel ($CoMo_3S_{13}$)	570	273	120, NA	13
$KFeSbS_3$	636	273	217, 60	14
$NaFeAsS_3$	505	273	188, 100	14
$KFeSbTe_3$	652	273	121, 75	This work

Table S3. Empirical parameters from fitting of virial equation in $KFeSbTe_3$.

Constant	CO_2	CH_4	H_2
Quantity absorbed (mmol/g)	1.356	0.0783	0.0488
Pressure (mmHg)	760	760	760
K (mmol/g/mmHg)	0.00562	7.07684×10^{-5}	4.26593×10^{-5}

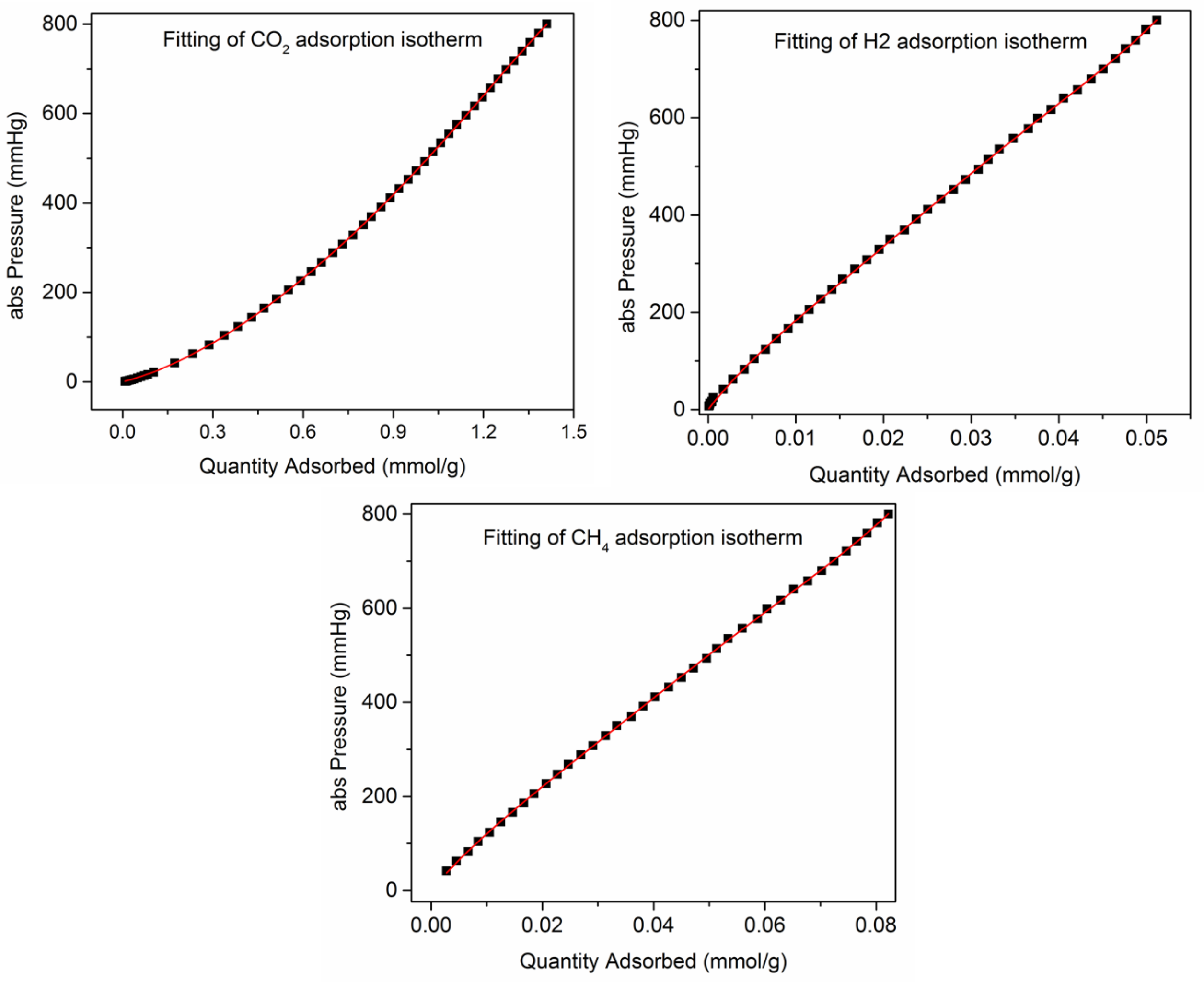
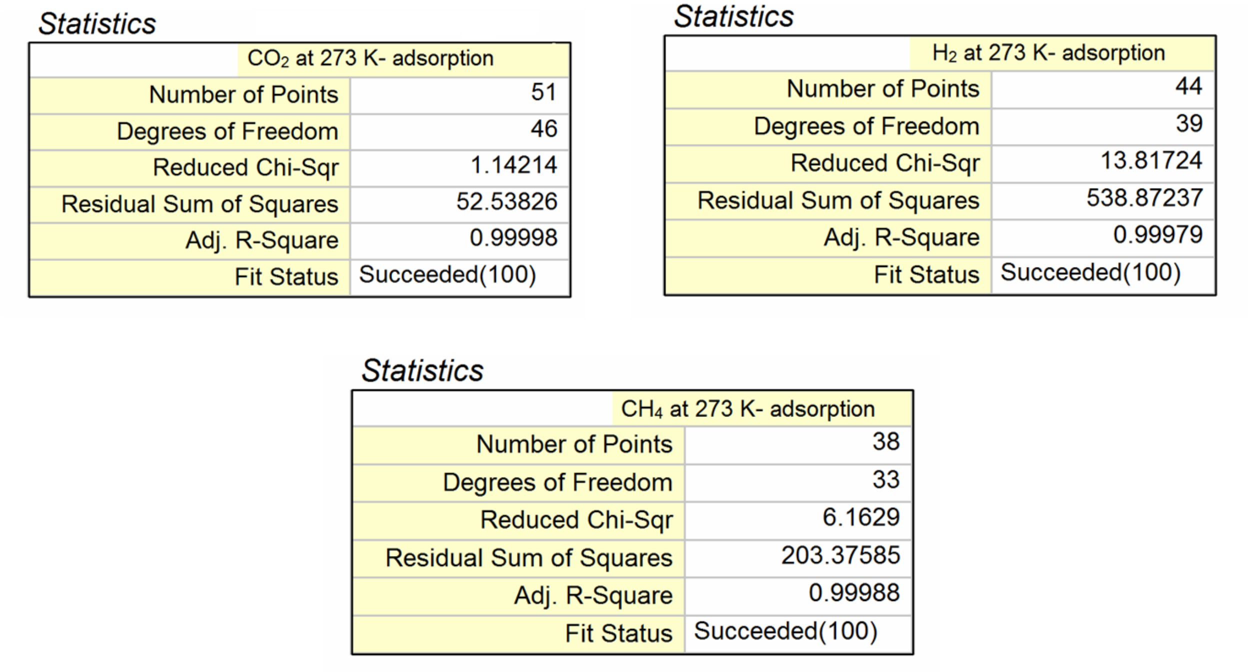


Figure S7: Fitting of Henry's constant for CO_2, CH_4 and H_2 in $KFeSbTe_3$ chalcogel.



Statistics

	CO_2 at 273 K- adsorption
Number of Points	51
Degrees of Freedom	46
Reduced Chi-Sqr	1.14214
Residual Sum of Squares	52.53826
Adj. R-Square	0.99998
Fit Status	Succeeded(100)

Statistics

	H_2 at 273 K- adsorption
Number of Points	44
Degrees of Freedom	39
Reduced Chi-Sqr	13.81724
Residual Sum of Squares	538.87237
Adj. R-Square	0.99979
Fit Status	Succeeded(100)

Statistics

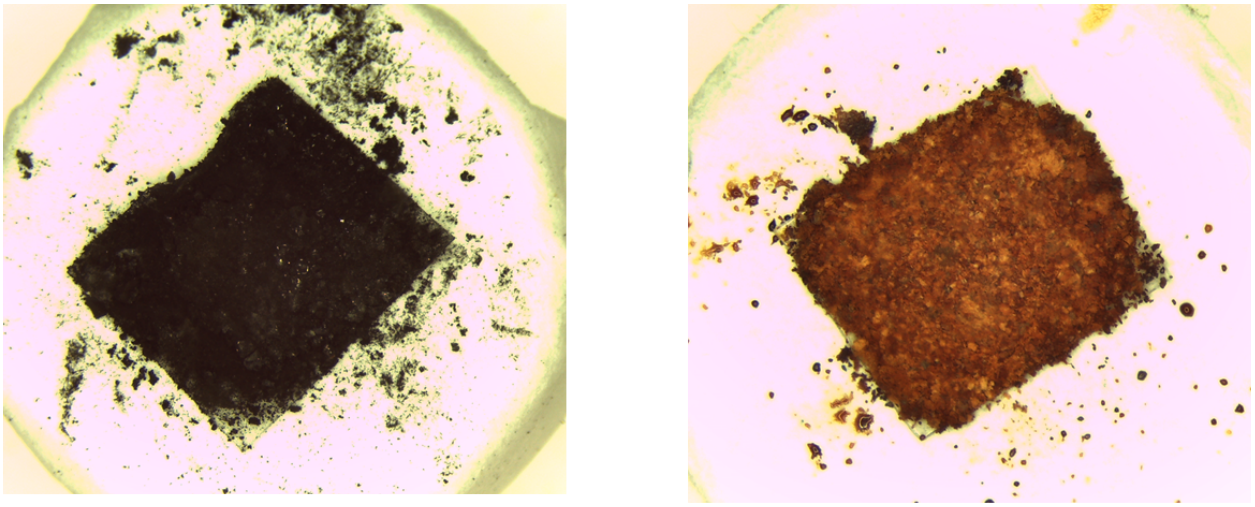
	CH_4 at 273 K- adsorption
Number of Points	38
Degrees of Freedom	33
Reduced Chi-Sqr	6.1629
Residual Sum of Squares	203.37585
Adj. R-Square	0.99988
Fit Status	Succeeded(100)

Figure S8: Statistics for the fitting of Henry's constant for CO_2, CH_4 and H_2 in $KFeSbTe_3$ chalcogel.

X-ray photoelectron spectroscopy (XPS)

The XPS studies of the powder samples were carried out in a Kratos Axis Ultra DLD spectrometer equipped with a monochromatic Al-Kα x-ray source (hν = 1486.6 eV) operating at 150 W, a multichannel plate and delay line detector under a vacuum of ~10^{-9} mbar. Measurements were performed in hybrid mode using electrostatic and magnetic lenses, and the take-off angle (angle between the sample surface normal and the electron optical axis of the spectrometer) was 0°. All spectra were recorded using an aperture slot of 300 μm×700 μm. The survey and high-resolution spectra were collected at fixed analyzer pass energies of 160 eV and 20 eV, respectively. Samples were mounted in floating mode in order to avoid differential charging. Charge neutralization was required for all samples. Binding energies were referenced to the sp^3 hybridized (C-C,C-H) carbon for the C1s set at 285.0 eV.

However, due to very air-sensitive nature of the chalcogel, the sample could not be handled at our experimental core facilities. This is demonstrated by the color change from black to dark brown during attempted XPS measurement (Supporting information, Fig S9-10). However, indirect evidence for Fe(II) was obtained by powder XRD after thermal analysis where FeTe was detected (Supporting information, Fig. S4).



KFeSbTe$_3$ before XPS

KFeSbTe$_3$ after XPS

Figure S9: Photographic illustration of KFeSbTe$_3$ chalcogel before and after XPS studies.

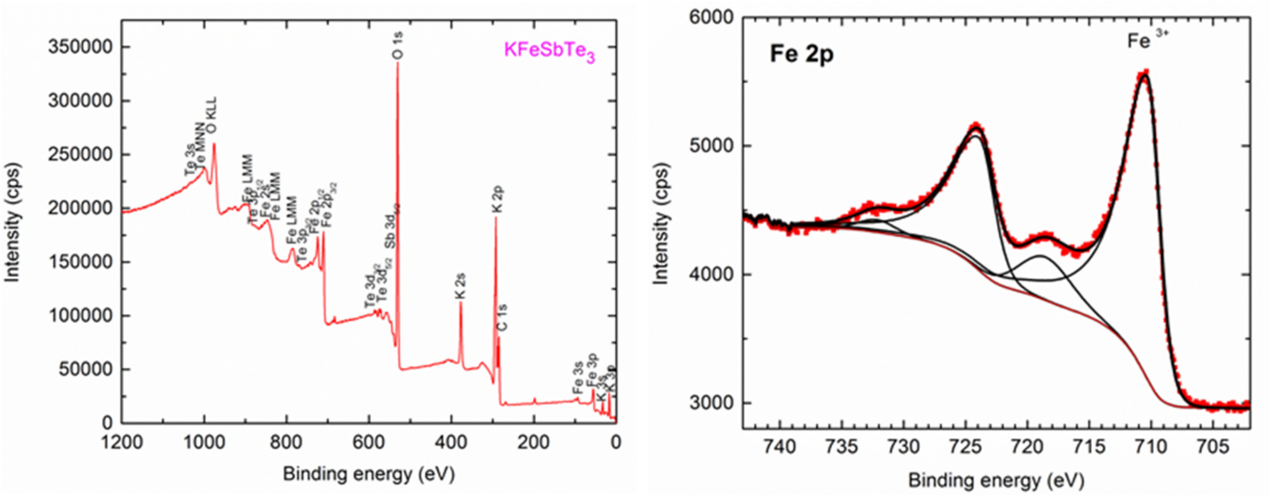


Figure S10: Left; Survey spectrum for the powdered **(decomposed)** chalcogel KFeSbTe$_3$ and right; high-resolution XPS spectrum of Fe 2p core level.

References:

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